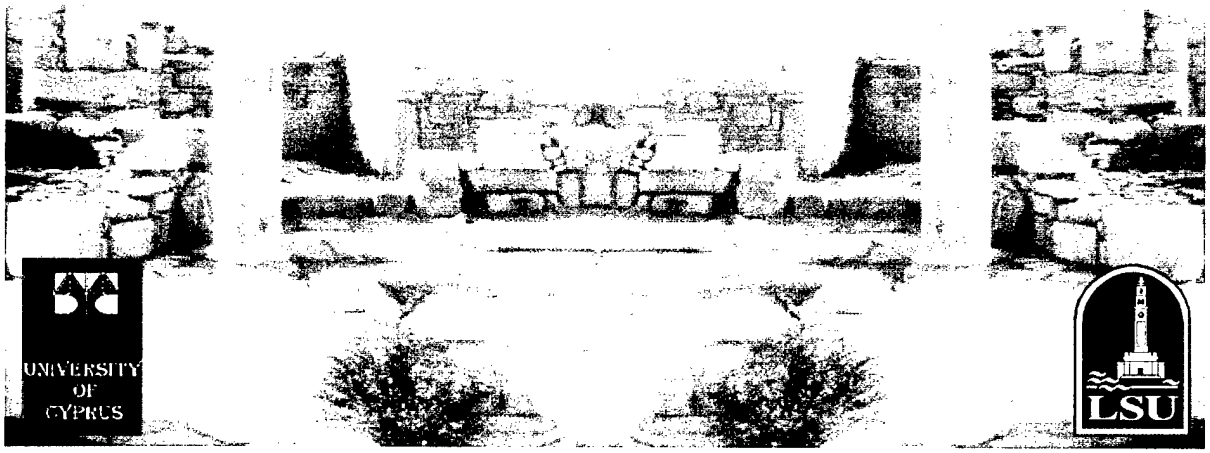

THE FIRST INTERNATIONAL CONFERENCE
ON
MULTISCALE MATERIALS PHENOMENA IN HARSH ENVIRONMENTS

JUNE 19 - 24, 2000

LIMASSOL, CYPRUS

BY

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INTERNATIONAL CONFERENCE
ON
MULTISCALE MATERIALS PHENOMENA IN HARSH ENVIRONMENTS

EXECUTIVE SUMMARY

We are seeking support to organize an international conference that will promote the confluence of ideas and expertise from diverse points of view in order to accelerate research on novel materials for harsh environments. The meeting will bring together experimental and computational materials scientists and engineers with expertise in atomistic and continuum approaches and grand challenge applications.

With the recent emergence of highly efficient multiresolution algorithms and massively parallel machines, materials simulation has reached a level of sophistication that can aid experimental efforts involving the synthesis of novel materials. At the present time it is possible to describe, with excellent accuracy, phenomena at the scale of nanometers using first-principles quantum mechanical calculations of the electronic structure. Semi-empirical approaches based on the tight-binding approximation provide an adequate description at length scales of tens of nanometers. Carefully parameterized interatomic potentials in conjunction with the molecular-dynamics method allow the successful description of systems on submicron length scales. Finally, finite-element approaches are successful in treating the large length scales relevant to the materials properties, provided the basic constitutive relations that include the effect of microstructural changes in the form of damage caused by external loading conditions are available. In addition, it is necessary to have a seamless coupling of simulation approaches at various length scales and time scales. The proposed conference will address this problem as well as other important simulation and experimental issues concerning multiscale materials phenomena.

The conference will be held from June 19-24, 2000 in Limassol, Cyprus. We expect 80-100 participants from academia and national and industrial laboratories. The conference format will include invited and contributed talks and poster sessions. The requested funds will partially cover the travel, local expenses and registration fee for the invited speakers; the costs of producing and mailing conference posters and other literature; and the audio/visual and other equipment-rental costs.

1 RATIONALE FOR PROPOSED CONFERENCE

Novel materials that can withstand extreme environments are generating considerable worldwide attention. Such materials are tremendously important for defense technologies. The basic requirements for designing materials depends crucially on the development of constitutive relations that include the effect of microstructural changes in the form of damage caused by external loading conditions.

The current search for such materials is largely based on traditional experimental methods. An effective way of accelerating research in this field is to have synergism between experiments, materials simulations, and high performance computing and communications (HPCC). This will greatly help experimental efforts involving the synthesis of novel materials for harsh environments. The proposed conference will foster such synergism between experimental and computational materials scientists/engineers and experts in HPCC.

2 SCIENTIFIC/ENGINEERING BACKGROUND

The quest for materials that can operate under extremely harsh conditions is one of the dominant themes in materials science and engineering. Despite a great deal of research, many perplexing problems remain concerning mechanical properties and thermal behavior of materials as well as environmental effects at high temperatures and stresses. Research in this area has thus far focused on controlling structures at diverse length scales -- atoms, defects, fibers, interfaces, grains, pores, etc. Because of the inherent complexity of such multiscale materials phenomena, computer modeling is expected to play an important role in the search for novel materials that can withstand extreme operating conditions. In recent years we have witnessed rapid progress in large-scale atomistic simulations, highly efficient algorithms for massively parallel machines, and immersive and interactive virtual environments for analyzing and controlling simulations in real time. Thus, materials simulations are capable of complementing and guiding experimental search for novel materials, provided the micro-, meso-, and macro-scale simulations can be coupled seamlessly.

The micro-mechanism and macro-mechanical modeling behavior of advanced materials need to be addressed. In particular, the

interrelationship between microstructural degradation and loading conditions need to be modeled and quantified. It encompasses the identification and interpretation of damage at different length scales and forms a micro-mechanical system where damage is assessed at the micro scale due to microcracks and microvoids in the material. It addresses damage due to debonding at the interface between different constituents of the material.

3 SCOPE OF THE CONFERENCE

The aim of the proposed conference is to provide experimental and computational materials scientists/engineers with a forum to exchange ideas and discuss the latest developments in multiscale phenomena in materials for harsh environments. The conference will focus on various thermo-mechanical aspects including deformation, the influence of large strains and strain rates, creep, fatigue, and dynamic fracture in these materials. The conference will feature recent developments in ab initio electronic structure calculations, large scale molecular-dynamics simulations based on reliable interactions, finite-element methods, parallel algorithms for materials simulations, and immersive and interactive visualization environments for virtual design of materials. The proposed conference is unique in that it will combine state-of-the-art multiscale modeling with recent experimental developments.

4 TOPICS

The proposed conference will feature oral and poster presentations on the following topics:

* Ceramics, composites, intermetallic compounds, and nanophase materials;
* Phase stability, thermal stability, oxidation resistance, and thermal shock resistance of materials at high temperatures and stresses, and high radiation;
* Measurements, modeling, and monitoring of residual stresses, growth of defects, effects of high strain and strain rates, creep behavior, fracture, and the effect of environment on materials;
* Ab initio electronic structure, molecular dynamics, Monte Carlo, and continuum approaches for material simulations;

* Theoretical formulation and computational implementation of multiple damage in materials;
* Non-local approaches to deformation in order to describe plastic instabilities including dislocation patterning and spatial characteristics of shear bands;
* Physically based solution for the lifetime predictions of structural components under specific load patterns.

5 APPEAL OF THE CONFERENCE

Federal agencies and various industries are investing heavily in research on materials that can withstand extreme operating conditions. Therefore, the proposed conference will attract a wide range of researchers from academia, government laboratories, and industries. We expect the participants will include experimental and computational material scientists and engineers, and experts in parallel algorithms and immersive and interactive virtual environments for the design of materials. The conference will attract researchers not only from the U.S., but also from Europe and Japan.

6 LOCATION, DATES, AND THE SIZE OF THE CONFERENCE

The conference will be held from June 19-24, 2000 at the Hawaii Hotel in Limassol, Cyprus. It will feature approximately 40 oral and 30 poster presentations. We expect 80-100 participants from materials science and engineering, condensed-matter physics, chemistry, and computational sciences.

7 CONFERENCE ORGANIZERS

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8 QUALIFICATIONS OF ORGANIZERS

The organizers have considerable experience in performing large-scale materials simulations, and detector monitoring on various parallel platforms. They have used molecular dynamics (MD), quantum molecular dynamics, variational Monte Carlo, and Green's Function Monte Carlo techniques to investigate material properties and processes. In recent years, they have designed highly efficient algorithms to carry out multimillion atom MD simulations on parallel machines. Currently they are investigating structural correlations, mechanical properties, thermal transport, and dynamic fracture in high-temperature ceramics, metal/ceramic composites, amorphous carbon and diamond films, micro-electro-mechanical-systems (MEMS), and nanophase materials. They are also designing novel materials-simulation techniques based on wavelets and other multiresolution approaches. Their research also includes work on damage characterization of materials with emphasis on theoretical modeling and experimental correlation. Research activities of particular interest encompass macro-mechanical/micro-mechanical constitutive modeling, experimental procedure for quantification of crack densities, inelastic behavior, thermal effects, interfaces, damage and fracture, failure, and numerical modeling. During the past five years, they have organized at least one international conference every year.

9 AGENDA

MONDAY MORNING, JUNE 19, 2000

REGISTRATION	8:00 AM – 9:00 AM
INTRODUCTION AND WELCOME	9:00 AM – 9:20 AM
John Zavada (ARO, USA)	9:20 AM – 10:00 AM
Dusan Krajcinovic (Arizona State University, USA) *Damage and Failure of Disordered Materials on Molecular, Micro and Macro Scales*	10:00 AM – 10:40AM
COFFEE BREAK	10:40 AM – 11:00 AM
Andrew M. Rappe (University of Pennsylvania, USA) *New Approaches to Modeling Complex Systems*	11:00 AM – 11:40 AM
David Pettifor (Oxford University, UK) *Bond-Order Potentials: Bridging the Electronic to Atomistic Modelling Hierarchies*	11:40 AM – 12:20 PM
K. Vasudevan (Office of Naval Research, USA) *A Unified Approach to Fatigue Crack Nucleation and Growth*	12:20 PM – 1:00 PM

MONDAY AFTERNOON, JUNE 19, 2000

COCKTAILS	4:00 PM – 4:30 PM
Thomas A. Weber (NSF, USA) *Materials Research at NSF and the FY 2001 US Government*	4:30 PM – 5:10 PM
Michael Berman (AFOSR, USA)	5:10 PM – 5:50 PM

TUESDAY MORNING, JUNE 20, 2000

Kirk C. Valanis (University of Portland, USA) *Quantum Plasticity*	9:00 AM – 9:40 AM
Armen Khachaturyan (Rutgers University, USA) *Modeling of Mesoscale and Microscale Microstructure Evolution*	9:40 AM – 10:20 AM
Khemais Saanouni (Univ. de Techn. de Troyes, France) *Numerical Simulation of Damage in Metal Forming Processes*	10:20 AM – 11:00 AM
COFFEE BREAK	11:00 AM – 11:30 AM
Socrates T. Pantelides (Vanderbilt University, USA) *Silicon MOSFETs: Atomic-Scale Structure and the Effect of Space Radiation*	11:30 AM – 12:10 PM

Sabine M. Schloegl (Delft Univ. of Techn., Netherlands) 12:10 PM – 12:50 PM
Microstructural Evolution During Hydrogenation in Low Cr-Mo Steels

TUESDAY AFTERNOON, JUNE 20, 2000

Carl Thompson (MIT, USA) 4:00 PM – 4:40 PM

Michael Plesha (University of Wisconsin, USA) 4:40 PM – 5:20 PM

Eiji Tsuchida (NIAIR, Japan) 5:20 PM – 6:00 PM
Adaptive Finite-Element Method for Electronic-Structure Calculations

WEDNESDAY MORNING, JUNE 21, 2000

Alexander Pechenik (AFOSR/NC, USA) 9:00 AM – 9:40 AM
Factors Causing Uncertainty in Properties and Performance of Modern Structural Materials

John P. Dempsey (Clarkson University, USA) 9:40 AM – 10:20 AM
The Fracture of Ice from Single Crystal to Geophysical Scale

Elisabeth Bouchaud (Saclay, France) 10:20 AM – 11:00 AM
Crack Fronts and Damage in some Complex Microstructures

COFFEE BREAK 11:00 AM – 11:30 AM

George Z. Voyiadjis (Louisiana State University, USA) 11:30 AM – 12:10 PM
Multi-scale Analysis of Multiple Damage Mechanisms in Composite Materials

Kaspar Willam (University of Colorado Boulder, USA) 12:10 PM – 12:50 PM
Failure Analysis of Materials and Structures at Different Levels of Observation

M. Zikry (North Carolina State University, USA) 12:50 PM – 1:30 PM
Global Failure and Microstructural Evolution in Porous Crystalline Aggregates

WEDNESDAY AFTERNOON, JUNE 21, 2000

EXCURSION 4:00 PM – 10:00 PM
Kourion Amphitheatre and Kolossi Castle or to Troodos Mountain

THURSDAY MORNING, JUNE 22, 2000

Renata M. Wentzcovitch (University of Minnesota, USA) 9:00 AM – 9:40 AM

George Frantziskonis (University of Arizona, USA) 9:40 AM – 10:20 AM
Compound Wavelet Matrix for Bridging Simulations at Complementary Scales - Application to Microstructure Evolution

Alex Hansen (Norwegian Univ. of Sc. and Techn., Norway) 10:20 AM –11:00 AM
Stress Distribution on Rough Surfaces in Contact

COFFEE BREAK 11:00 AM – 11:30 AM

Aiichiro Nakano (Louisiana State University, USA) 11:30 AM – 12:10 PM
Multiresolution Simulations of Nanostructured Solids

Chun Loong (Argonne National Lab, USA) 12:10 PM – 12:50 PM
Proton and Electron Conduction in Yttrium-Doped Barium Cerate Ceramics under a Hydrogen-Containing Atmosphere at High Temperatures

THURSDAY AFTERNOON, JUNE 22, 2000

Ruth Pachter (Wright Lab, USA) 4:00 PM – 4:40 PM

Gerald H. Lushington (OSC/PET-CCM, USA) 4:40 PM – 5:20 PM

Kenji Tsuruta (Okayama University, Japan) 5:20 PM – 6:00 PM
Parallel Tight-Binding Molecular Dynamics of Nanostructured Ceramics

Dimitris Papaconstantopoulos (NRL, USA) 6:00 PM – 6:40 PM
Tight-Binding Method: Connections to First-Principles and to Molecular Dynamics

CONFERENCE BANQUET 8:00 PM – 11:00 PM

FRIDAY MORNING, JUNE 23, 2000

Elias C. Aifantis (Aristotle Univ. of Thessaloniki, Greece) 9:00 AM – 9:40 AM
Multiscale Models of Deformation: Wavelets and Size Effects

Sadasivan Shankar (Intel Coorp. USA) 9:40 AM – 10:20 AM
Multiple Length and Time Scale Modeling of Materials Processing

Shuji Ogata (Yamaguchi University, Japan) 10:20 AM – 11:00 AM
Formative Processes of Oxide Scales on Aluminum Nanoparticles: Variable-Charge Molecular Dynamic on Parallel Computers

COFFEE BREAK 11:00 AM – 11:30 AM

Martina E. Bachlechner/Elefterios Lidorikis (LSU, USA) 11:30 AM – 12:10 PM
Multiscale Simulations of Electronic Devices

Hiroshi Iyetomi (Niigata University, Japan) 12:10 PM – 12:50 PM
Molecular Dynamics Study on the Microscopic Structure of Doped Oxide Glasses

FRIDAY AFTEROON, JUNE 23, 2000

Hussein M. Zbib (Washington State University, USA) 4:00 PM – 4:40 PM
Multi Scale Approach for Deformation and Fracture

Laurent Van Brutzel (Louisiana State University, USA) 4:40 PM – 5:20 PM
Study of Crack Propagation Mode in Silica and Nanophase Silica by Molecular Dynamics Simulations

SATURDAY MORNING, JUNE 24, 2000

Fuyuki Shimojo (Hiroshima University, Japan) 8:00 AM – 8:40 AM
Molecular Dynamics Simulation of Structural Phase Transition in Silicon Carbide

Andrei Artemev (Carleton University, USA) 8:40 AM – 9:20 AM
The Phase Field Model and Computer Simulation of Proper Martensitic Transformation in Fe-Ni and Ti-Ni Alloys

Raffaello D'Alessandro (INFN-Sezione di Firenze, Italy) 9:20 AM – 10:00 AM
Silicon Tracker: Detector Performance in a High Radiation Environment

SATURDAY AFTERNOON, JUNE 24, 2000

EXCURSION 10:30 AM – 8:30 PM
Paphos

MULTISCALE MODELS OF DEFORMATION: WAVELETS AND SIZE EFFECTS

Elias C.Aifantis

Laboratory of Mechanics and Materials, Polytechnic School
Aristotle University of Thessaloniki
Thessaloniki, 54006 Greece

Various higher order models of elasticity, dislocation dynamics and plasticity are reviewed. Their implications to a variety of heterogeneity and patterning phenomena not captured by classical models are discussed and a number of interesting engineering problems are solved. Then, emphasis is placed on the physical interpretation of the new gradient terms, the corresponding extra boundary conditions and the determination of the relevant gradient coefficients. Finally, the role of wavelet analysis in bridging length scales and interpreting size effects is discussed.

THE PHASE FIELD MODEL AND COMPUTER SIMULATION OF MARTENSITIC TRANSFORMATION IN FE-NI AND TI-NI ALLOYS

Andrei Artemev*, Y. Jin and A.G. Khachaturyan

*Department of Mechanical and Aerospace Engineering, Carleton University, 1125 Colonel By Dr., Ottawa, Ontario, K1S 5B6 Canada

Department of Ceramic and Materials Engineering, Rutgers University, 607 Taylor Rd., P.O. Piscataway, New Jersey 08854, U.S.A.

The three dimensional phase field model of the martensitic transformation has been developed. The evolution of phase field functions is described by a kinetic equation of Ginsburg-Landau type, which explicitly takes into account the contribution of the transformation-induced coherency strain by using the phase field micromechanics of a structurally inhomogeneous coherent system. This model has been used to simulate the fcc to bcc transformation in Fe - 31.0 at. % Ni alloys and cubic B2 phase to trigonal R phase transformation in Ti - 50.0 at. % Ni alloys. Simulations were performed for the wide range of undercoolings and under both constrained and unconstrained conditions for an average deformation in the systems. A microstructures with polytwinned martensite structures were obtained under constrained conditions. A large value of the volumetric transformation effect in Fe - 31.0 at. % Ni system resulted in significant fractions of the residual parent phase after the transformation. The volume fraction of the residual parent phase in this system depended strongly on undercooling. The simulation under unconstrained conditions produced two types of structure. In one case, a single crystal structure with only one martensite orientation variant was obtained. In the other case, the structure can be described as the system of parallel layers of two different orientation variants.

MULTISCALE SIMULATIONS OF ELECTRONIC DEVICES

Martina E. Bachlechner, Ingvar Ebbsjö*, Rajiv K. Kalia, **Elefterios Lidorikis**, Anupam Madhukar**, Aiichiro Nakano, Priya Vashishta, George Z. Voyiadjis***, and Phillip Walsh

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The interface structure and stress distribution in Si(111)/a-Si_3N_4 nanopixels are studied using molecular dynamics (MD) simulations on parallel computers. Bulk Si is described by the Stillinger-Weber potential and Si_3N_4 is represented by a combination of two- and three-body interactions that include steric, charge transfer, polarizability, and covalent forces. The charge transfer at the interface is extracted from self-consistent LCAO electronic structure calculations. The MD simulations for Si(111)/a-Si_3N_4 nanopixels involve different pixel sizes with systems consisting of up to 27 million atoms. In all these systems, we find stress domains at the interface which persist into the silicon substrate. The nature of the stress domains will be discussed.

We have also developed a scheme in which the physical system is divided into FE, MD, and handshake (HS) regions. The HS and FE regions are far away from process zones. Within the MD region, the dynamics of atoms is governed by suitable potentials as described above, while in the FE region the equations for continuum elastic dynamics are solved on a computational grid. To ensure smooth transition, the dynamics obeyed by hybrid atoms/nodes in the HS region are governed by the average Hamiltonian of the MD and FE schemes. Stresses in Si(111)/Si_3N_4(0001) nanopixels will be presented.

CRACK FRONTS AND DAMAGE IN SOME COMPLEX MICROSTRUCTURES

Elisabeth Bouchaud*, Florin Paun**, and Elodie Ducourthial***

*SRSIM, CEA-SACLAY, FRANCE
**DMMP, ONERA, FRANCE
***DMSE, ONERA, FRANCE

The study of the morphology of fracture surfaces has raised a great theoretical interest in the past few years. Although qualitatively satisfactory, models describing the propagating crack front as an elastic string moving through randomly distributed microstructural obstacles have failed to predict the actual roughness exponents characterizing fracture surfaces. The very basic assumptions of this category of models is questioned, and the importance of damage created during crack propagation is emphasized. A different scenario taking place at intermediate length scales is proposed, based on experimental observations and on numerical simulations. Experimentally, the morphology of damage cavities is explored, and it is shown that cavities independent of the main crack have the same self-affine properties as fracture surfaces at small length scales. The non trivial roughness exponent 0.8 observed at larger length scales is conjectured to be linked to strong correlations of damage. As a matter of fact, numerical simulations on a model material composed of brittle precipitates likely to break in cleavage in an elastic matrix show that the correlation length of cracks does correspond to the multi-cracked zone size. Strong correlations are shown to be present between damage microcracks, forcing the main crack to progress along a path which is clearly not a simple directed random walk.

SILICON TRACKER: DETECTOR PERFORMANCE IN A HIGH RADIATION ENVIRONMENT

Raffaello D'Alessandro
(for the CMS silicon tracker collaboration)

Dipartimento di Fisica
INFN-Sezione di Firenze,
Largo E. Fermi 2, I-50125 Firenze, ITALY

The problematic concerning the use of silicon sensors in a hostile environment, such as that present at LHC, will be presented. Although the conditions might seem prohibitive, the R&D work done by our collaboration has shown that silicon sensors can nonetheless still be employed for tracking purposes provided appropriate care is taken in their use. I will show how the performance degrades and what counter measures can and will be taken so that the tracker will continue to satisfy the CMS requirements during its whole lifetime. I will also review the implications of, the recently approved, all silicon tracker and the developments in silicon detector technology that have made feasable such a large surface detector.

THE FRACTURE OF ICE FROM SINGLE CRYSTAL TO GEOPHYSICAL SCALE

John P. Dempsey

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An understanding of the fracture behavior of ice is sought at many scales. The lab-scale brittle failure of ice under compression is accompanied by a plethora of cracking scenarios, as are the structural-scale interactions of ice sheets with offshore structures, ships, icebreakers, coastal structures, submarines and tankers. At the mesoscale, the accurate incorporation of ridging, rafting and lead formation into constitutive models is seen as critical to the determination of ice strength on a geophysical scale. On a planetary scale, venusian tectonics appears to more closely resemble the ridges and leads in convergent field of arctic pack ice, while there is reason to believe that an understanding of sea-ice processes can provide insight into the complex geology of Europa. All of the above phenomena involve the fracture of ice at varying scales and at extremely high homologous temperatures. The influence of scale on both creep and fracture has been explored through experiments via self-similar experiments scaled from 1:160. The issue of scale and its influence on both the constitutive and fracture behavior of ice is hugely important to the fields of ice dynamics and ice mechanics.

COMPOUND WAVELET MATRIX FOR BRIDGING SIMULATIONS AT COMPLEMENTARY SCALES - APPLICATION TO MICROSTRUCTURE EVOLUTION

George Frantziskonis

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and

P. A. Deymier

Materials Science and Engineering
University of Arizona
Tucson, AZ 85721

We introduce a wavelet-based compound matrix that allows bridging simulations performed at various spatial and time scales. We apply this method to the phenomenon of normal grain growth. In the particular application addressed herein molecular dynamics simulations are combined with Monte Carlo ones of a lattice Q-states Potts model. The compound wavelet matrix formed from the two types of simulation provides full statistical information on material properties at the range of scales that is the union of those handled by the two methods.

STRESS DISTRIBUTION ON ROUGH SURFACES IN CONTACT

Alex Hansen

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Norwegian University of Science and Technology
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(In collaboration with G. George Batrouni, INLN, Universite de Nice and Jean Schmittbuhl, Ecole Normale Superieure, Paris)

The stress distribution on the surface of elastic materials in contact plays an important role in determining their frictional properties. We report here on recent numerical studies of elastic media in contact where their surfaces are rough [1]. The roughness is assumed to be self affine, that is, length scales orthogonal to the surface scales with length scales in the surface with an exponent H. Fracture surfaces have this property.

We also report on some entirely unexpected scaling properties for self affine surfaces in a range of exponent H which is relevant to describe the stress field [2].

[1] A. Hansen, J. Schmittbuhl and G. G. Batrouni, "Normal Stress Distribution of Rough Surfaces in Contact," submitted to Geophys. Res. Lett.

[2] A. Hansen, J. Schmittbuhl and G. G. Batrouni, "istinguishing Fractional and White Noise in One and Two Dimensions," to be submitted to Phys. Rev. Lett.

MOLECULAR DYNAMICS STUDY ON THE MICROSCOPIC STRUCTURE OF DOPED OXIDE GLASSES

Hiroshi Iyetomi

Department of Physics
Niigata University
Ikarashi, Niigata 950-2181, Japan

The network structure of oxide glasses such as B2O3, SiO2 and GeO2 consists of basic building units in which the network-forming cations are threefold or fourfold coordinated by oxygen ions (triangle for B2O3; tetrahedron for SiO2 and GeO2). Medium-range order with a characteristic length beyond the nearest-neighbor distances thus emerges as a result of structural correlations among those basic units. The first sharp diffraction peak in the static structure factor reflects the medium-range order in the glassy network. Doping even a slight amount of impurities into the monolithic glasses can drastically change their material characteristics. The purpose of the present study is to elucidate modification of the network structure of the glasses caused by incorporation of metal oxides (Li2O, Na2O) through molecular dynamics (MD) simulations. The interatomic interactions in the simulations are described by a pairwise Born-Mayer-Huggins potential with electric charges and repulsive energy parameters alone. Comparison with neutron scattering experiments demonstrates essential features of the structural properties of the glasses are reproduced in such a simple ionic model. A doped metal ion has two possible roles as a network modifier in the glassy networks. It first promotes structural change of the building units to polydedra with higher coordination number, leading to increase of the network coherence. Its second role is to terminate connection of the units associated by formation of non-bridging oxygen. The MD simulations clarify which role the metal ion plays in a given multi-component glass.

PROTON AND ELECTRON CONDUCTION IN YTTRIUM-DOPED BARIUM CERATE CERAMICS UNDER A HYDROGEN-CONTAINING ATMOSPHERE AT HIGH TEMPERATURES

C.-K. Loong, J. W. Richardson, Jr., and U. Balachandran

Intense Pulsed Neutron Source Division and Energy Technology Division
Argonne National Laboratory
Argonne, Illinois 60439-4814, U. S. A.

Y-doped BaCeO3 exhibits high proton conducting properties under a hydrogen-containing atmosphere at high temperatures. This system has high potential for applications as fuel-cell electrolytes, gas sensors, and ceramic membranes for hydrogen separation, which require the exposure of the materials under harsh environments. In order to meet the technological demands for high efficient and cost-effective performance, the ceramic needs to be dense and nonporous, mechanically and chemically stable, highly selective to hydrogen, and catalytically active under a pressure gradient of reducing atmosphere at high temperatures up to 900°C. A successful development of these novel materials requires an understanding of their microscopic properties over a wide range of length and energy scale - from electronic response to atomic diffusion to crystal phases to microstructures. We have performed in-situ neutron diffraction to obtain information regarding the crystal phase evolution that accommodates the dissolution of hydrogen and proton migration through the lattice. Neutron quasielastic and inelastic-scattering experiments were carried out to investigate the hopping and vibrations of hydrogen via OHΣO sites near oxygen vacancies.

Work performed at Argonne National Laboratory is supported by the U. S. DOE-Basic Energy Science and Federal Energy Technology Center under the contract No. W-31-109-ENG-38.

Int,l Mtg on High-Temperature Materials, Maui, 1999

MULTIRESOLUTION SIMULATIONS OF NANOSTRUCTURED SOLIDS

Aiichiro Nakano, Paulo S. Branicio, Timothy J. Campbell, Ingvar Ebbsjo, Rajiv K. Kalia, Hideaki Kikuchi, Sanjay Kodiyalam, Xinlian Liu, Shuji Ogata, Andrey Omeltchenko, Jose P. Rino, Fuyuki Shimojo, Xiaotao Su, Priya Vashishta, and Phllip Walsh

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To perform 10-100 million-atom molecular-dynamics (MD) simulations of nanostructured materials and nanodevices, we have developed space-time multiresolution algorithms with adaptive load balancing for massively parallel machines, immersive and interactive visualization schemes, and efficient data management and mining approaches. Scalability of the MD algorithms involving up to 1.02 billion atoms has been tested on 1,024 Cray T3E processors under a DoD Challenge project.

Application of these algorithms to Grand Challenge MD simulations of properties and processes in a number of nanostructured materials and nanoscale devices will be discussed. Work supported by NSF, DOE, AFOSR, USC-LSU Multidisciplinary University Research Initiative, ARO, and NASA.

FORMATIVE PROCESSES OF OXIDE SCALES ON ALUMINUM NANOPARTICLES: VARIABLE-CHARGE MOLECULAR DYNAMIC ON PARALLEL COMPUTERS

Shuji Ogata,* Rajiv K. Kalia,+ Timothy J. Campbell,+ Aiichiro Nakano,+ and Priya Vashishta+

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Molecular dynamics simulations for oxidation of aluminum nanoparticles (radius, 100 Angstrom) in molecular oxygens have been performed on parallel computers using an adaptive interatomic potential capable of describing bond formation and breakage processes. In the potential, effective atomic-charges vary dynamically depending on the environment. Among other findings we observed saturation of the surface oxide thickness after 35 picoseconds [T.J. Campbell, R.K. Kalia, A. Nakano, P. Vashishta, S. Ogata, and S. Rodgers, Phys. Rev. Lett. Vol. 82, p. 4866 (1999)]. Through detailed analyses on the microscopic structures of the surface oxides, we discover a rapid three-stage process that leads to the saturation behavior in 50 picoseconds. In the first 5 picoseconds, oxygen molecules dissociate, and the atoms diffuse into octahedral and subsequently into tetrahedral sites in the Al nanoparticle. In the next 20 picoseconds fraction of four-fold coordinated oxygen atoms (OAl4) increases dramatically, which form isolated clusters of corner-sharing and edge-sharing tetrahedra. A neutral, percolating tetrahedral network forms between 30 and 35 picoseconds. As a result, a stable oxide scale is formed. The thickness and structure of the surface oxides are in accordance with experimental results.

SILICON MOSFETS: ATOMIC-SCALE STRUCTURE AND THE EFFECT OF SPACE RADIATION

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First-principles calculations have been used to identify the key atomic-scale mechanisms that underlie the oxidation of Si, the formation of interface defects, and the preference for abrupt and smooth interfaces. Space radiation has been known to induce several modes of degradation whose atomic-scale origin is still unclear. New calculations track several possibilities and relate them to observations.

TIGHT-BINDING METHOD: CONNECTIONS TO FIRST-PRINCIPLES AND TO MOLECULAR DYNAMICS

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Tight-binding total energy methods can be used as a link between highly accurate, but slow and memory consuming, first-principles density functional calculations and fast, compact, but less accurate atomistic potential methods.

We have constructed tight-binding(TB) Hamiltonians which are used to interpolate between the first-principles results, allowing accurate determinations of structural energy orderings, elastic constants, phonon frequencies, and surface energies. We have also developed computer programs which can use the TB parameters to do tight-binding molecular dynamics for the study of temperature-dependent properties. Our method is successful for a variety of materials including both metals and semiconductors as well as magnetic systems.

This work is supported by the U.S. Office of Naval Research and the Department of Defense Common HPC Software Support Initiative (CHSSI) program.

BOND-ORDER POTENTIALS: BRIDGING THE ELECTRONIC TO ATOMISTIC MODELLING HIERARCHIES

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Novel analytic bond-order potentials (BOPs) are derived for atomistic simulations by coarse graining the electronic structure within the orthogonal two-centre tight-binding (TB) representation. We show that these BOPs allow the concept of single, double, triple and conjugate bonds in carbon systems to be quantified, so that they provide the first 'classical' interatomic potentials that handle both structural differentiation and radical formation naturally within their remit. Finally, we show that this recently-developed BOP formalism allows us to derive explicit, analytic expressions for the environmental dependence of the TB bond integrals, applying the theory to the high-temperature intermetallic MoSi2.

NEW APPROACHES TO MODELING COMPLEX SYSTEMS

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Solid solutions provide unique properties which are inaccessible in pure materials. Ferroelectric materials are one of many important areas in which small changes in atomic composition dramatically change material properties. Theoretical examinations have been hampered by the difficulty of incorporating inhomogeneities into perfectly periodic systems. Several theoretical approaches have been formulated to address this specific issue, including the virtual crystal approximation (VCA), with only modest success.

We have overcome significant shortcomings of the standard VCA by developing a potential which yields averaged atomic properties; our designed nonlocal pseudopotential approach plays a key role in this process. We perform the VCA on a ferroelectric oxide, determining the energy differences between the high-temperature rhombohedral, low-temperature rhombohedral and tetragonal phases of $Pb(Zr1\text{-}xTix)O_3$ at various compositions and comparing these results to previously reported superlattice calculations and experiment. This work represents the first ab initio determination of a compositional phase boundary in an oxide solid solution.

NUMERICAL SIMULATION OF DAMAGE IN METAL FORMING PROCESSES

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Ductile (or plastic) damage often occurs during metal forming processes due to the large plastic flow localisation. Accordingly it is crucial for numerical tools, used in the simulation of that processes, to use fully coupled constitutive equations accounting for both hardening and damage. This can be used in both cases, namely to overcome the damage initiation during some metal forming processes as forging, stamping, deep drawing, ... or to enhance damage initiation and growth as in sheetmetal cutting or machining ....

In this talk, a fully coupled constitutive equations accounting for both combined isotropic and kinematic hardening as well as the ductile damage is implemented into the general purpose Finite Element code for metal forming simulation. First, the formulation of the fully coupled anisotropic constitutive equations in the framework of Continuum Damage Mechanics is presented. The particular case of the fully isotropic and isothermal flow is presented in details concerning both the plastic flow and the damage. The associated numerical aspects concerning both the local integration of the coupled constitutive equations as well as the (global) equilibrium integration schemes are presented. For fully implicit resolution strategy, a special care is given to the consistent stiffness matrix calculation and the reduction of the number of the constitutive equations within an implicit asymptotic integration scheme. For dynamic explicit resolution strategy, the adaptive control of the time step is discussed within the same implicit local integration scheme. The numerical implementation of the damage is made in such a manner that calculations can be executed with or without damage effect, i.e. coupled or uncoupled calculations.

Many numerical results are presented to discuss the capability of the model to predict the damage initiation and growth during the metal forming processes. For some examples, a comparison between coupled and uncoupled solutions are made using both : fully explicit and fully implicit " global " schemes. Applications are made to the numerical simulation of various 3D metal forming processes as hydroforming of tubes, forging of a spider or deep drawing of a square box.

MICROSTRUCTURAL EVOLUTION DURING HYDROGENATION IN LOW CR-MO STEELS

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Hydrogen attack is a material degradation process that occurs in steel components (e.g. pressure vessels) when they are exposed to high pressures of hydrogen at elevated temperatures. During this process, the dissolved hydrogen reacts with the carbides of the steel to form methane inside grain boundary cavities. Hydrogen attack involves several interacting processes including diffusion of H, C and of the metal atoms; dissolution of carbides; reaction of C with H to methane; dislocation creep and grain boundary diffusion.

A microstructural model is presented which takes into account the above-mentioned processes within the framework of a multi-component, multi-phase continuum description. We start with a ferritic matrix containing M_7C_3 and M_6C carbides. As a first step, the diffusion-controlled microstructural change of such a Fe-Cr-Mo-C steel due to temperature exposure is studied. Then, the model is applied to predict the microstructural evolution, the growth of cavities and the resulting methane pressure during hydrogen exposure. The simulations show that in many cases cavity growth and methane generation are strongly coupled, thus falsifying previous decoupled approaches to hydrogen attack.

MOLECULAR DYNAMICS SIMULATION OF STRUCTURAL PHASE TRANSITION IN SILICON CARBIDE

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We have carried out isothermal-isobaric molecular-dynamics (MD) simulations to understand the microscopic mechanism of the pressure-induced phase transition in silicon carbide. The effective interatomic potential in MD simulations consists of two- and three-body terms. The parameters in the potential are optimized so that the lattice constant, bulk moduli, cohesive energy, etc. are in accordance with experimental data. The melting or decomposition temperature and the phonon density-of-states obtained by MD simulations are found to be in good agreement with experiments. High-pressure MD simulations reveal a transformation from a four-fold coordinated zincblende structure to a six-fold coordinated rocksalt structure with a 15-20 % volume contraction and a decrease in the Si-C distance from 1.9 Å to 1.7 Å. These results along with the calculated transition pressure are in excellent agreement with experiments. The simulation also reveals that the MD cell is deformed from cubic to monoclinic, and Si- and C-sublattices are displaced in the (100) direction in such a way that the six-fold coordination occurs without any bond breaking.

ADAPTIVE FINITE-ELEMENT METHOD FOR ELECTRONIC-STRUCTURE CALCULATIONS

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We present a method of electronic-structure calculations which is based on the combination of density-functional theory and the finite-element method [1]. The performance of our method is enhanced significantly by several techniques, e.g. the adaptive curvilinear coordinates and the multigrid method. Our method is also suited for massively parallel computing. We show a number of recent applications including the semiconductor surfaces [2] and molecular liquids [3]. Future extensions of this approach are also surveyed.

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PARALLEL TIGHT-BINDING MOLECULAR DYNAMICS OF NANOSTRUCTURED CERAMICS*

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Atomistic and electronic structures of nanocstructured ceramics are investigated by an order-N tight-binding molecular dynamics (TBMD) method. We have employed the Fermi-operator expansion strategy [1] for calculations of electronic energy and forces, which scales linearly with respect to the system size. Parallel PC clusters, connected via a gigabit switch, have been used for a benchmark of the code and TBMD simulations. We have performed TBMD simulations of sintering of nanocrystalline SiC (grain size ~ 2-3nm) at high temperatures (1000 1500K) [2]. We show effects of grain orientation on the sintering processes. Surface reconstruction prior to the neck formation affects significantly structures in the grain boundary. Analyses via Mulliken scheme for local electronic population and density-of-states show grain boundary structures and their effects on gap states of the sintered SiC systems. The order-N TB method has been extended to efficient calculation of electrical conductivity [3]. Preliminary results for dc conductivity of the nanocrystalline SiC will also be presented.

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QUANTUM PLASTICITY

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Currently, quantum behavior is associated with systems of atomic dimensions. Such systems may occupy only one energy level in a (discrete) spectrum which is determined by the solution of the Schrodinger Equation, specific to that particular system.

It has been observed for some time that material systems of phenomenological dimensions under stress, exhibit similar behavior in the sense that all inelastic (plastic) states, or a subset thereof, appear spontaneously in an unstable fashion and exist only at discrete values of the surface tractions. Here, it is shown that these states and the corresponding tractions, are also determined by an equation similar to that of Schrodinger. We call this equation the Quantum Instability Equation. This equation is derived in the text from principles of gradient thermodynamics originated by the author. Close agreement between the theoretical values of the "quantum tractions" and their experimental counterparts is demonstrated for several experiments.

A UNIFIED APPROACH TO FATIGUE CRACK NUCLEATION AND GROWTH

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A 'unified' approach to fatigue crack growth has been developed using two driving force parameters. It has been shown that the crack growth involves two thresholds, one in terms of DK and the other Kmax. These two thresholds have to be satisfied simultaneously for crack growth to occur.

The anamolous behavior of short cracks,acceleration/retardation due to overloads/underloads have been successfully accounted using the two parametric driving force approach. Using the classic Kitagawa diagram, one can clearly show the crack nucleation and growth regions can be combined to give a physically meaningful and self-consistant 'unified' frame work for the the overall fatigue damage. Finally, the role of 'internal stresses' in crack nucleation, short carcks, over and underloads are discussed in the framework of the 'unified' damage approach.

MULTI-SCALE ANALYSIS OF DAMAGE COUPLED WITH INELASTIC BEHAVIOR IN COMPOSITE MATERIALS

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The proposed work introduces gradients at both meso and macroscale. The combined coupled concept of introducing gradients at the mesoscale and macroscale enables one to address two issues simultaneously. The mesoscale gradients allow one to address issues such as lack of statistical homogeneous state variables at the macroscale level such as debonding of fibers in composite materials, crack, voids, etc. On the other hand the macroscale gradients allow one to address non local behavior of materials and interpret the collective behavior of defects such as dislocations and cracks.

In this work an attempt is made to introduce damage and plasticity internal state variables at both the macro and mesoscale levels in order to provide sufficient of defects and their interaction to properly (i.e. physically) characterize the material behavior. This will provide an adequate characterization of these defects in terms of size, orientation, distribution, spacing, interaction among defects, etc. In order to achieve this the bridging of multiple scales need to be addressed and implemented properly. The gradient of these internal state variables will be also incorporated in order to address the non local effects. An attempt to expand this bridging to micro-scale level is too computationally prohibitive for the immediate future.

The internal state variables will be categorized into two groups, one that is statistically homogeneous at the representative volume element (RVE) and the other which can only be statistically homogeneous at a subvolume of the RVE. For an RVE made of two phase materials the defects in each constituent and the interphase (debonding) cannot be categorized as statistically homogeneous for the RVE unless a very low order measure of these defects is used to characterize damage or plasticity. The RVE implied here is matrix with a single fiber in the middle of the RVE. The subvolumes characterization of damage and plasticity at a level below the RVE allows one to adequately characterize the details of these defects.

MATERIALS RESEARCH AT NSF AND THE FY 2001 US GOVERNMENT

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This talk will discuss Materials Research Programs funded by the US National Science Foundation. In addition, the talk will focus on the NSF and government-wide initiatives proposed by President Clinton in his FY 2001 Budget to Congress. Specifically, the talk will discuss the Information Technology Research Initiative and the National Nanotechnology Initiative as they impact material science and engineering researchers.

FAILURE ANALYSIS OF MATERIALS AND STRUCTURES AT DIFFERENT LEVELS OF OBSERVATION

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In 'Failure Analysis' we address deterioration mechanisms which start in the small, at multiple scales of the material point, and which propagate onto the large, when progressive failure of a structural component or an entire structural system is considered. This progression of failure mechanisms at different levels of observation is exacerbated and accelerated by harsh environments comprised of mechanical and environmental effects such as dynamic impact loading and hygro-thermo-chemical attack.

In the presentation we will review some of the fundamental failure diagnostics which are being used at the material level to indicate continuous and discontinuous failure in the small. Subsequently, we investigate their extension onto the level of structural components and systems. Specifically, we will resort to spectral techniques to examine deterioration in two- and three-phase particulate material systems which are discretized via finite elements and homogenized at the macro level. Hereby, our specific interest will be the effect of interfacial debonding and slip on the overall integrity of the composite.

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GLOBAL FAILURE AND MICROSTRUCTURAL EVOLUTION IN POROUS CRYSTALLINE AGGREGATES

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A multiple-slip dislocation-density based constitutive formulation and specialized computational schemes have been developed to characterize material failure on the appropriate physical scales needed for the accurate prediction of physical mechanisms that control failure initiation, growth, and coalescence. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and tilt orientations. These evolving local stress fields are used as failure criteria to track the initiation and evolution of intergranular and transgranular fracture. The interrelated effects of grain boundary orientation, dislocation density pile-ups and evolution, geometrical and thermal softening, void distribution and geometry, and hydrostatic stresses on failure paths in cubic crystalline materials have been studied.